Ethanimidic acid, N-hydroxy-, ethyl ester

105/6-12-2	D1XSID2065129	

Model Performance

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Model	II)ata
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Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 2.70

Global applicability domain: Inside

Local applicability domain index: 9.88e-01

Confidence level: 8.15e-01

Nearest Neighbors from the Training Set

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Ethyl acetate Measured: 2.70 Predicted: 2.70

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2-Methylpropanenitrile Measured: 2.87 Predicted: 2.60

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Formic acid, propyl ester Measured: 2.66 Predicted: 2.80

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Methyl ethyl ketone Measured: 2.71 Predicted: 2.80

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(Z)-1,2-Dichloroethylene

Measured: 2.56 Predicted: 2.81